9,12,15-Octadecatrienoic acid

Other names: Octadeca-9,12,15-trienoic acid
Inchi: InChI=1S/C18H30O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(19)20/h3-4,6-7,9-1
InchiKey: DTOSIQBPPRVQHS-IUQGRGSQSA-N
Formula: C18H30O2
SMILES: CCC=CCC=CCC=CCCCCCCCC(=O)O
Mol. weight [g/mol]: 278.43
CAS: 1955-33-5

Physical Properties

Property code	Value	Unit	Source
gf	75.60	kJ/mol	Joback Method
hf	-328.00	kJ/mol	Joback Method
hfus	48.67	kJ/mol	Joback Method
hvap	78.96	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	5.661		Crippen Method
mcvol	259.020	ml/mol	McGowan Method
pc	1440.25	kPa	Joback Method
rinpol	2125.00		NIST Webbook
rinpol	2117.00		NIST Webbook
rinpol	2117.00		NIST Webbook
ripol	3554.00		NIST Webbook
tb	769.77	K	Joback Method
tc	951.83	K	Joback Method
tf	388.13	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.47	J/mol×K	769.77	Joback Method
cpg	832.74	J/mol×K	921.49	Joback Method
cpg	819.88	J/mol×K	891.14	Joback Method
cpg	806.48	J/mol×K	860.80	Joback Method

cpg	792.49	J/mol×K	830.46	Joback Method
cpg	777.83	J/mol×K	800.11	Joback Method
cpg	845.11	J/mol×K	951.83	Joback Method
dvisc	0.0000155	Pa×s	769.77	Joback Method
dvisc	0.0000245	Pa×s	706.16	Joback Method
dvisc	0.0000423	Pa×s	642.56	Joback Method
dvisc	0.0000823	Pa×s	578.95	Joback Method
dvisc	0.0001891	Pa×s	515.34	Joback Method
dvisc	0.0005488	Pa×s	451.74	Joback Method
dvisc	0.0022584	Pa×s	388.13	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1955335&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume